UNRAVELLING THE CHEMICAL COMPLEXITY OF ESSENTIAL OILS: IN-DEPTH CHARACTERIZATION AND PROFILING BY GC×GC-MS

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INTRODUCTION

Essential oils are characterized by the presence of numerous compounds belonging to different chemical classes, with a variety of key aroma compounds being present at different concentration levels. Gas chromatography coupled to mass spectrometry (GC-MS) is often employed for their analysis, however resolution is not sufficient to unravel such elevated complexity. Detailed characterization remains challenging at best, in particular for the determination of low-level compounds potentially significant for their impact on sensory properties.

Comprehensive two-dimensional gas chromatography (GC×GC) offers significantly enhanced separation power and superior peak capacity. It can therefore play a strategic role to tackle high complexity with elevated degree of detail. In this study GC×GC, combined with the additional dimension added by MS data, was employed for untargeted profiling of chemical composition of rosemary and lavender leaf essential oil.

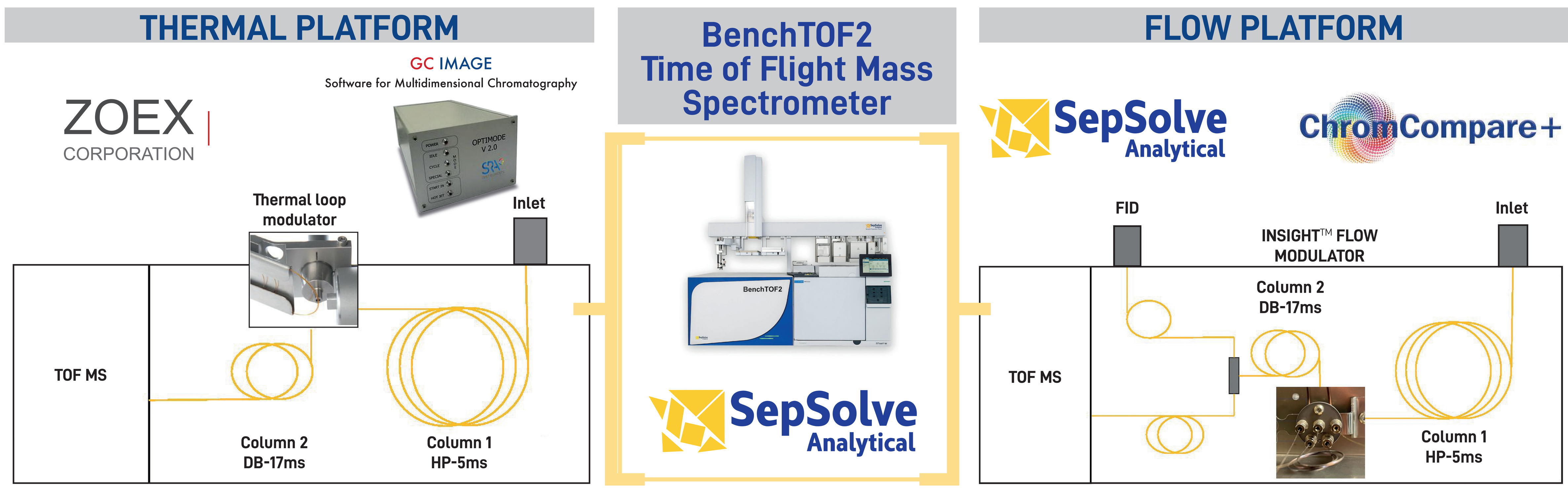
GOALS

- Investigated the chemical composition of lavender and rosemary leaf oils from plants harvested in Italy produced by steam extraction in small batches.
- Commercial products were analysed to evaluate the impact of isolation process.
- Analyses were performed by GC×GC-TOFMS based on flow and thermal modulation, respectively.
- Data processing performed with commercial software, including statistical tools such as Principal Component Analysis (PCA), was used for sample classification.

EXPERIMENTAL

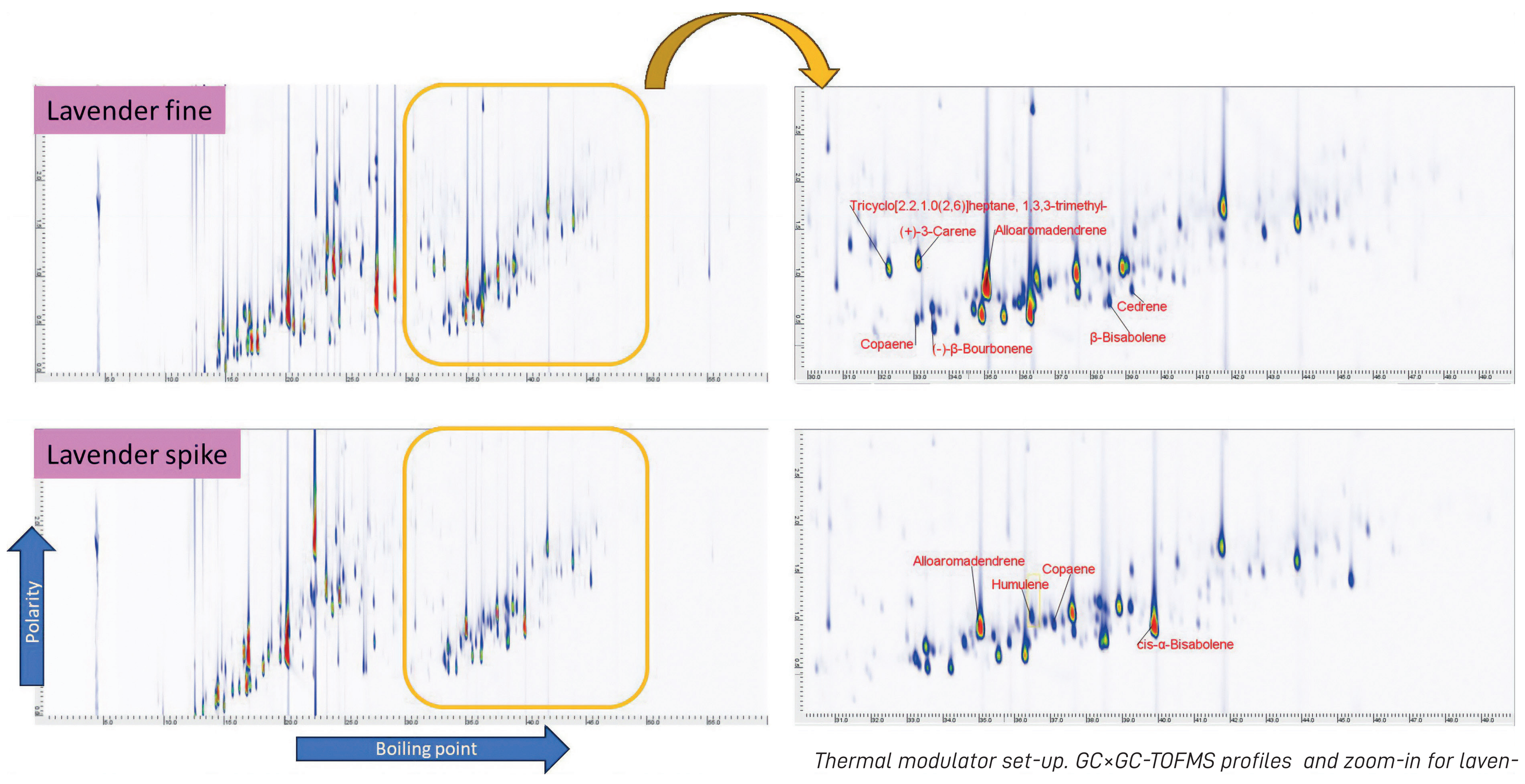
SAMPLES

- Plants: lavender *(Lavandula Officinalis L. Angustifolia Miller – or Spica – and Lavandula Officinalis L. - or Fine)* and rosemary *(Rosmarinus Officinalis L. Camphoriferum and Rosmarinus Officinalis L. Verbenoniferum).*
- Essential oils were obtained by steam distillation with production on a small scale. Water was brought to a boil to generate a steam current that was directed through the plant material (leaves) to release the oil.
- After condensation to liquid phase, the aqueous phase was discharged by gravity and the organic phase was collected as the final product.

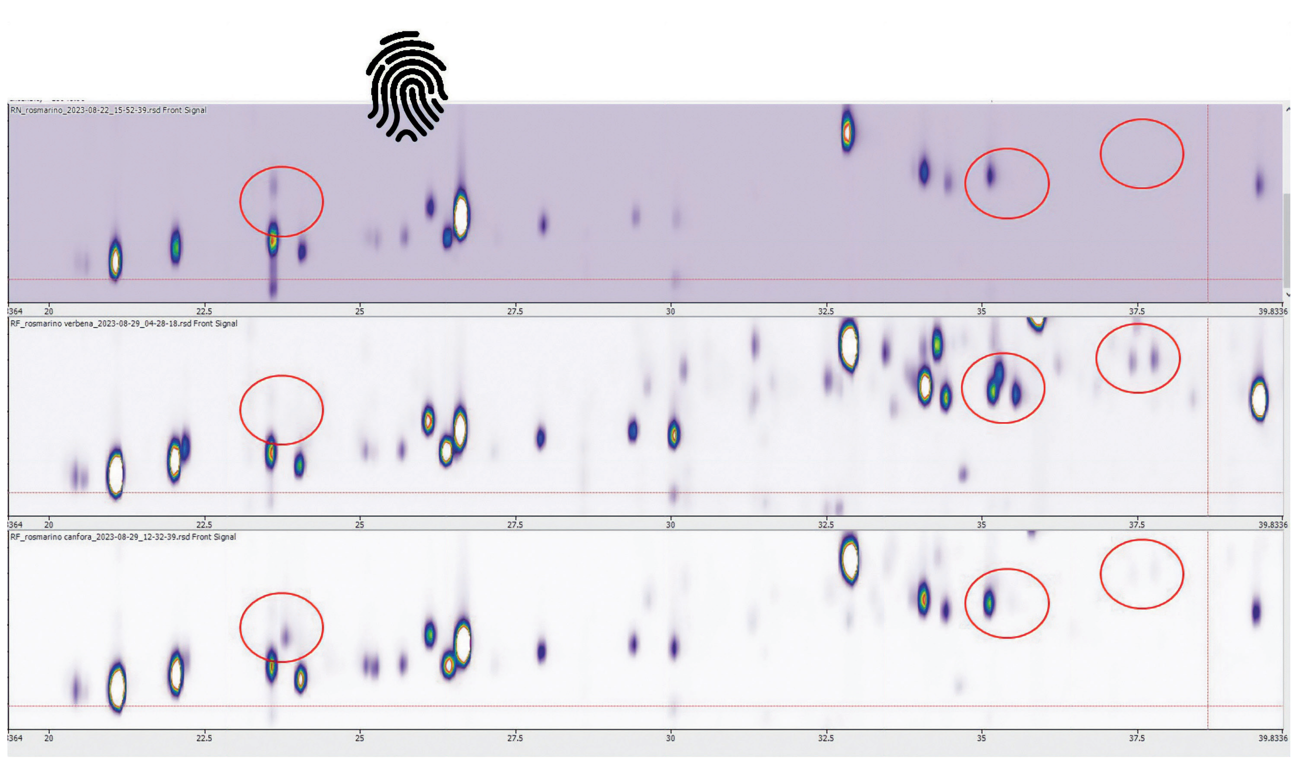


RESULTS

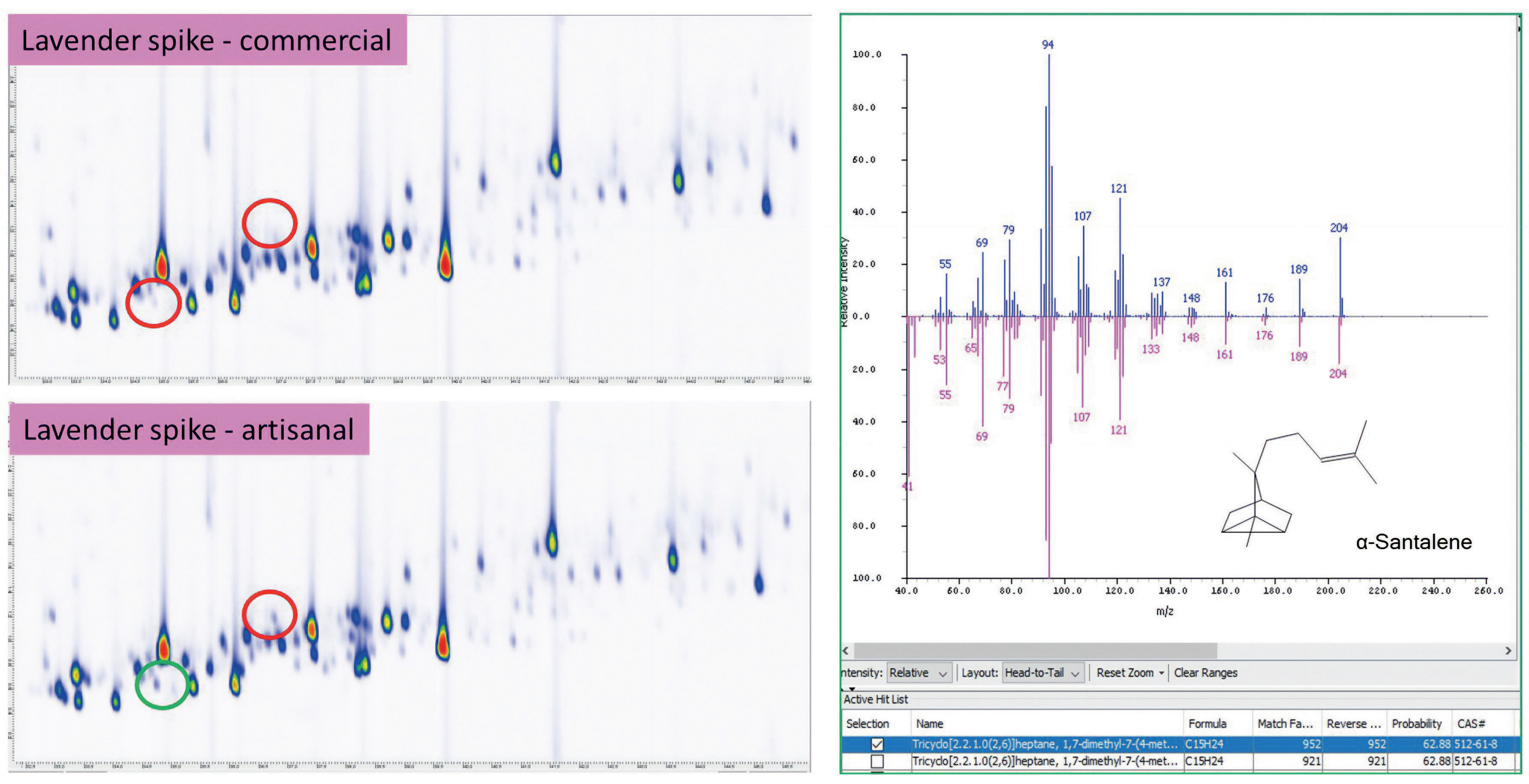
- GC×GC-MS allowed effectively separating and detecting a significantly higher number of components compared to conventional GC-MS.
- Individual compounds and chemical groups were distributed across a 2D space, reducing co-elutions. Cleaner spectra are beneficial to improve the identification process, bringing value added for untargeted screening.
- Informative 2D chromatograms confirmed excellent for samples comparison. Differences in composition between lavender and rosemary oils from different strains were observed. Similarly, it was possible to discover differences between essential oils produced by small-scale approach and the commercial oils.
- The streamlined workflows offered by the data processing software allowed to minimize laborious, challenging procedures to enable advanced yet (semi-)automated user-friendly operation.



Thermal modulator set-up. GC×GC-TOFMS profiles and zoom-in for lavender essential oils from different plant strains.

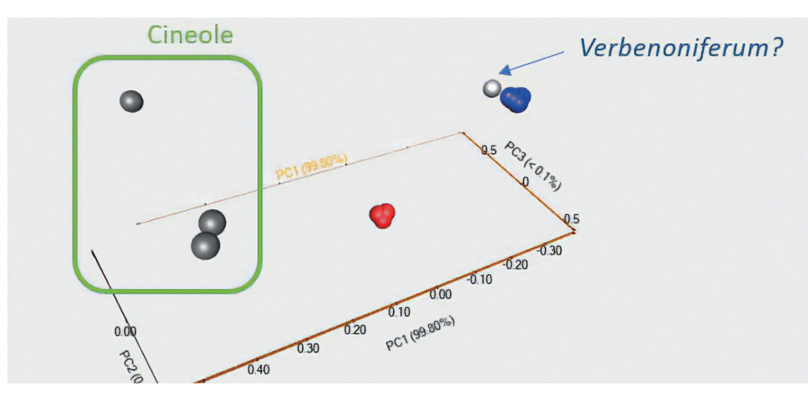


Flow modulator set-up. 2D FID plots for rosemary essential oils from different plant strains. Even without the identification capability of MS data, 2D profiles allow effective comparison by fingerprinting useful for classification.

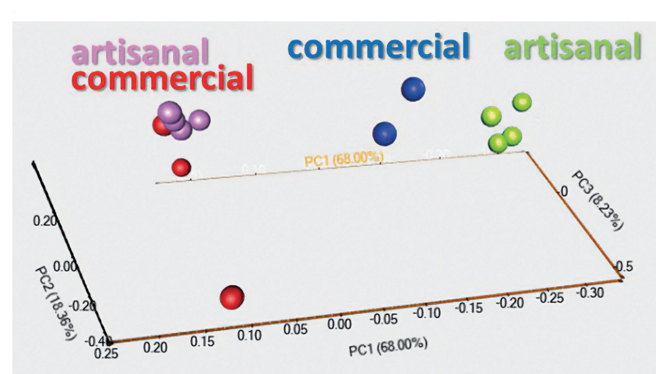


Thermal modulator set-up. GC×GC-TOFMS of lavender essential oils from the same plant strain. Chromatograms refer to small-batch in-house oil and a commercial product, respectively. A selective trace-level peak is fully separated from more predominant components and identified with good reliability by direct MS library search.

Examples of classification by PCA (ChromCompare+ software, SepSolve Analytical) based on TOFMS data acquired with the flow-modulated set-up.



Classification of rosemary oils from different plant strains.
Blue: Rosmarinus Verbenoniferum; red: Rosmarinus Camphoriferum; Gray: unknown commercial samples.



Classification of lavender oils from different plant strains and production.
Red/pink: Lavandula Officinalis L. Angustifolia Miller (SPICA);
Blue/green: Lavandula Officinalis L. (FINE).

CONCLUSIONS

- GC×GC-MS is a very powerful tool for detailed profiling of complex mixtures such as essential oils.
- Chemical composition of lavender and rosemary oils was characterized with much more insight compared to conventional separation techniques.
- Characteristic 2D profiles demonstrated very effective to highlight differences useful to classify origin in terms of plant strains pr production.
- The multivariate analysis tools employed proved useful to extend the applicability of advanced data processing in an effective yet accessible manner.

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